

# Universality of subleading corrections for self-avoiding walks in presence of one-dimensional defects

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## Abstract

We study three-dimensional self-avoiding walks in presence of a one-dimensional excluded region. We show the appearance of a universal sub-leading exponent which is independent of the particular shape and symmetries of the excluded region. A classical argument provides the estimate:  $\Delta = 2\nu - 1 \approx 0.175(1)$ . The numerical simulation gives  $\Delta = 0.18(2)$ .

# 1 Introduction

An important problem in statistical mechanics is the study of the critical behaviour of systems in geometries with boundaries. One usually considers situations in which the geometric constraint changes the critical behaviour: in the renormalization-group terminology these are the cases in which the boundary is a *relevant* perturbation. However there are also cases, as the one we are concerned with in this paper, in which the leading critical behaviour is unchanged and the presence of the boundary appears as an *irrelevant* perturbation.

Maybe because of their name the role of *irrelevant* operators is generally not well studied. Indeed, by definition, they do not modify the fixed point of the renormalization-group transformations. In particular they do not change the values of the critical exponents and manifest themselves only through subleading corrections to the fixed-point hamiltonian. Nonetheless in any actual computation the fixed-point hamiltonian is replaced by an effective hamiltonian whose parameters are tuned closed to criticality. This means that as soon as a precise determination of the universal scaling behaviour is needed, it becomes important to have good control also on the terms responsible for corrections to scaling.

In this paper, we will concentrate on three-dimensional self-avoiding walks (SAWs) in presence of an excluded one-dimensional region. We will extend the results of [1, 2, 3] which showed for the case of a half-line the appearance of a new critical exponent  $\Delta \approx 0.22$ . Here we will consider more general one-dimensional regions and we will show that the value of  $\Delta$  is independent of the shape and symmetries of the excluded region: only the dimensionality plays a role. Moreover we will show that  $\Delta$  can be predicted to a very good accuracy by a purely geometrical argument.

The paper is organized as follows: in Section 2 we give a general discussion of the relevance of the perturbation introduced by the excluded region and we give a prediction for the subleading exponent. In Section 3 we describe the geometries we analyze and the choice of observables which allow the easiest and most precise determination of  $\Delta$ . In Section 4 we give a few details of the simulation, while in Section 5 we give the final results. Appendix A presents the computation of the generating function for ordinary random walks in presence of excluded hyperplanes which allow a direct check of the results of Section 2. An analogous computation for the case a single excluded point and for an excluded needle is reported in [1]. Appendix B contains some unrelated results on the small-momentum behaviour of the two-point function.

## 2 Excluded set and corrections to scaling

In the terminology of the field-theoretic approach to critical phenomena, the critical behaviour of the SAW is governed by the fixed-point of the  $O(n)$   $\sigma$ -model analytically continued to  $n = 0$  [4, 5, 6, 7, 8, 9]. The presence of an excluded region corresponds to a perturbation due to the introduction of an operator which creates vacancies in

the  $O(n)$  model. Now consider the correlation function<sup>1</sup> between a spin at the origin and one in the bulk at location  $\vec{r}$ ; this function will have the scaling form

$$G_{\mathcal{R}}(\vec{r}; \beta) \sim r^{-(d-2+\eta_{\mathcal{R}})} F_{\mathcal{R}}(\vec{r}/\xi(\beta)) + r^{-(d-2+\eta'_{\mathcal{R}})} F'_{\mathcal{R}}(\vec{r}/\xi(\beta)) + \dots \quad (2.2)$$

Here  $\beta$  is the inverse temperature, and  $\xi \sim (\beta_c - \beta)^{-\nu}$  is the correlation length *in the unperturbed theory*; the critical inverse temperature  $\beta_c$  and the exponent  $\nu$  are *not* modified by the presence of the vacancies, unless the excluded region  $\mathcal{R}$  is so big that the remaining set  $\mathbf{Z}^d \setminus \mathcal{R}$  is effectively a space of lower dimensionality. See Ref. [10] for how thin a set has to be before  $\mu = 1/\beta_c$  changes. However, the behaviour of the other quantities depends on whether the perturbation is relevant or irrelevant [11]:

- (a) If the perturbation is *relevant*, then the leading spin-spin decay exponent  $\eta_{\mathcal{R}}$  *differs* from its bulk value  $\eta$  [and as a consequence the leading susceptibility exponent  $\gamma_{\mathcal{R}} = (2 - \eta_{\mathcal{R}})\nu$  differs from its bulk value  $\gamma = (2 - \eta)\nu$ ]. Likewise, the leading scaling function  $F_{\mathcal{R}}$  differs from its bulk value  $F$ ; in particular, it has a non-trivial angular dependence [12].
- (b) If the perturbation is *irrelevant*, then  $\eta_{\mathcal{R}}$  and  $F_{\mathcal{R}}$  are *unchanged* from their bulk values  $\eta$  and  $F$ . In particular, the leading scaling function  $F$  has *no angular dependence*. The effects of the perturbation show up only in the *non-leading* exponents and scaling functions  $\eta'_{\mathcal{R}}, \dots$  and  $F'_{\mathcal{R}}, \dots$ , which *can* differ from their bulk values.

In either case,  $\eta_{\mathcal{R}}$  and  $F_{\mathcal{R}}$  (and indeed all of the exponents  $\eta'_{\mathcal{R}}, \dots$  and scaling functions  $F'_{\mathcal{R}}, \dots$  except for an unknown amplitude) are universal in the sense that they depend only on the *global* properties of the excluded region  $\mathcal{R}$ , such as its dimensionality.

More subtle is the case in which the perturbation is marginal:  $\eta_{\mathcal{R}}$  is equal to the bulk value but the universal scaling behaviour may be broken by logarithmic violations and observables associated to the perturbation can show a complete breaking of universality, in the sense that they can have critical exponent with an explicit dependence from the coupling of the perturbation [13, 14].

To understand the effect of the introduction of the excluded region we must thus understand if the perturbation is relevant or irrelevant. We will resort to a geometric argument. Consider in a  $d$ -dimensional space a set  $E$  and let  $d(E)$  denote the number of dimensions in which the set  $E$  extends to infinity. Let us now recall the fundamental rule in geometric probability for the dimension of the generic intersection  $A \cap B$  of two geometric sets  $A$  and  $B$  which are immersed in a space of  $d$  dimensions:

$$d(A \cap B) = d(A) + d(B) - d \quad . \quad (2.3)$$

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<sup>1</sup>In the SAW language we have

$$G_{\mathcal{R}}(\vec{r}; \beta) = \sum_{N=0}^{\infty} \beta^N c_{N,\mathcal{R}}(\vec{r}) \quad (2.1)$$

where  $c_{N,\mathcal{R}}(\vec{r})$  is the number of SAWs going from 0 to  $\vec{r}$  in  $N$  steps without intersecting the region  $\mathcal{R}$ .

A negative sign of  $d(A \cap B)$  means that  $A$  and  $B$  do not generically intersect in dimension  $d$  outside any bounded volume. The application of (2.3) extends also to random geometries where one considers a probability measure on a configuration space which is concentrated on a set of events with given Hausdorff dimension.

For example, the generic intersection of two ordinary random walks, which have Hausdorff dimension 2, has dimension  $4-d$ , and thus they do not generically intersect in  $d > 4$ . By using the well-known random-walk representation of the euclidean  $O(n)$ -vector field theory [15, 16, 8], for which the interaction is concentrated on the intersections among walks, it is then possible to understand why for  $d > 4$  in the critical region only a trivial theory is recovered: simply because the walks intersect almost nowhere! We can say that for  $d > 4$ :

- a) the probability of intersections of two random walks in the critical region scales towards its limiting value with the correlation-length as  $\xi^{4-d}$ ;
- b) critical indices take their free-field (that is mean-field) values, the interaction term in the hamiltonian is *irrelevant* and induces only sub-leading corrections.

In  $d = 4$  the interaction becomes *marginal* and is responsible only for logarithmic corrections to the critical indices [7]. It is said that 4 is the upper critical dimension of the model.

In  $d < 4$  the interaction is *relevant* and thus it changes the critical indices.

Similar ideas have been used to discuss the critical behaviour of gauge theories and random surfaces, see for example [17].

Let us now consider the case of walks in presence of an excluded region  $\mathcal{R}$  of dimension  $d_{\mathcal{R}}$ . Consider first ordinary random walks whose Hausdorff dimension is two. Then the dimension of a generic intersection with the region  $\mathcal{R}$  of dimension  $d_{\mathcal{R}}$  is

$$d_{int} = 2 + d_{\mathcal{R}} - d \quad (2.4)$$

The previous argument suggests the following cases

- $d_{\mathcal{R}} = 0$ : this is the case in which we are excluding only a finite set of lattice sites. The upper critical dimension (with its logarithmic corrections) is  $d = 2$ ;
- $d_{\mathcal{R}} = 1$ : this is the case in which we are excluding a finite set of one-dimensional lines. The upper critical dimension (with its logarithmic corrections) is  $d = 3$ .

Formula (2.4) can also be obtained from other considerations [1]. If  $\mathcal{R}$  is a  $d_{\mathcal{R}}$ -dimensional hyperplane, consider the projection of the walk on  $\mathcal{R}'$ , the orthogonal complement of  $\mathcal{R}$ . Also the projection is a random walk. The probability of intersection will be then the probability of first return to the point  $\mathcal{R} \cap \mathcal{R}'$ . But the probability that a  $\bar{d}$ -dimensional random walk eventually passes through a point scales as  $1/N^{\bar{d}/2-1}$  if  $\bar{d} > 2$ , while it is one if  $\bar{d} \leq 2$ . Since in our case  $\bar{d} = d - d_{\mathcal{R}}$ , we see that for  $d_{int} \geq 0$  the walk generically intersects the region  $\mathcal{R}$ , while for  $d_{int} < 0$  the probability vanishes as  $1/N^{-d_{int}/2}$ , in agreement with our argument. Finally notice that when  $d_{\mathcal{R}} = d - 1$ , one can apply the results for the so-called vicious walkers.

Indeed the behaviour of  $d$  one-dimensional vicious walkers<sup>2</sup> can be viewed as the behaviour of a  $d$ -dimensional walker in a space bounded by  $d(d-1)/2$   $(d-1)$ -dimensional hyperplanes [18, 19].

Let us now arrive at the case of SAW. Their Hausdorff dimension is  $1/\nu$  (see for example [7, Appendix B]). For the dimension of a generic intersection with the region  $\mathcal{R}$  we get

$$d_{int} = \frac{1}{\nu} + d_{\mathcal{R}} - d \quad (2.5)$$

Let us consider once more a series of cases, remembering that for  $d \leq 4$  according to the Flory formula  $\nu \approx 3/(d+2)$ , which is exact in  $d = 1, 2$ , must be corrected by logarithmic violations in  $d = 4$ , and is a good approximation in  $d = 3$ .

- $d_{\mathcal{R}} = 0$ : Excluded points are a relevant perturbation only if  $d \leq 1/\nu$ , that is in  $d = 1$ . We remark that the sub-case in which the excluded set consists of a single point  $\mathcal{R} = \mathcal{P}$ , when  $\mathcal{P}$  is chosen to be a nearest-neighbour of the origin of the walk, can be mapped into a problem *without* vacancies. Indeed each walk of  $N$  steps, starting from the origin, can be seen as a walk of  $N + 1$  steps starting from  $\mathcal{P}$  whose first step is the previous origin. Under this mapping the asymmetry induced by the exclusion of  $\mathcal{P}$  can be seen as the correlation between the position of the end-point of the walk with the direction of the first step.
- $d_{\mathcal{R}} = 1$ : in  $d = 1, 2$  the perturbation is relevant, but it is already irrelevant in  $d = 3$ .

Thus in  $d = 3$  with a finite set  $\mathcal{R}$  of excluded lines, we expect that, regardless of their disposition in space, the probability that a walk intersects the region  $\mathcal{R}$  scales as  $\xi^{2-1/\nu}$ , or, since  $\xi \sim N^\nu$ , as  $N^{2\nu-1}$ .

In the field-theoretic language this dimensional argument implies in (2.2)

$$\eta' = \eta - d_{int} = \eta + 2 - \frac{1}{\nu} \quad (2.6)$$

Consequently, if  $P_k(x)$  is a homogeneous polynomial of degree  $k$  in the coordinates of the end-point of the walk, we have

$$\langle P_k(x) \rangle_{N, \mathcal{R}} = N^{k\nu} \left( A(k) + \frac{B_{\mathcal{R}}(k)}{N^\Delta} + \dots \right) \quad (2.7)$$

where  $\langle \cdot \rangle_{N, \mathcal{R}}$  is the average in the ensemble of walks of length  $N$  that do not intersect  $\mathcal{R}$  and  $\Delta$  a subleading exponent. If (2.6) holds, we have

$$\Delta = -d_{int}\nu = 2\nu - 1 \quad (2.8)$$

In general we expect renormalization effects to change (2.6) and thus (2.8) introducing an anomalous dimension. However experience with three-dimensional models

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<sup>2</sup> Related work on vicious walkers can be found in Ref. [20, 21].

indicates that these corrections, if not vanishing, are extremely small and thus we expect (2.8) to be in any case a very good approximation.

The amplitude  $A(k)$  is not universal, because of an unknown scale factor, but it should not depend on the excluded region. Moreover, since in the critical limit the distribution of the end-point is rotationally symmetric,  $A(k)$  vanishes whenever  $\int d\Omega_x P_k(x) = 0$  where  $d\Omega_x$  is the normalized measure on the sphere  $S^{d-1}$ . This suggests a very convenient way to compute the subleading exponent  $\Delta$  induced by the introduction of the excluded region. The idea is to consider observables which have zero expectation value in the rotationally-invariant continuum limit and which do not vanish under the residual discrete symmetry that the lattice has after the introduction of the excluded region. For these quantities  $A(k) = 0$  so that the leading term scales as  $N^{k\nu-\Delta}$  which makes the determination of  $\Delta$  much easier. Let us notice that in all this discussion we have always assumed that the first subleading exponent is related to the introduction of the excluded region. This is true for those quantities for which  $\langle P_k(x) \rangle$  would vanish in absence of the excluded region, i.e. for those  $P_k(x)$  which are not only non-rotationally invariant but which are also not symmetric under the transformations of the cubic group. If instead  $\langle P_k(x) \rangle$  would not vanish even in absence of the excluded region, it is not clear a priori which exponent should show up first. For cubic-symmetric  $P_k(x)$  for which  $A(k) = 0$  an extensive analysis [22, 23] shows that in absence of any excluded region

$$\langle P_k(x) \rangle \sim N^{k\nu-\Delta_{latt}} \quad (2.9)$$

with  $\Delta_{latt} \approx 2\nu$ . For  $d = 3$  this exponent is much larger than (2.8) and thus, in presence of an excluded region, we expect all non-rotationally invariant  $P_k(x)$  to behave as  $N^{k\nu-\Delta}$  with  $\Delta$  given by (2.8). We should also mention that the exponent  $\Delta$  defined here is unrelated to the exponent  $\omega\nu \approx 0.5$  which controls the leading confluent correction for SAWs in absence of any excluded region and which has been the object of much attention in the literature [24, 25, 26, 27].

### 3 The models

We have concentrated upon the problem of 3- $d$  SAWs starting from the origin in presence of an excluded region  $\mathcal{R}$  which consists of a finite collection of half-lines — we will call them “*needles*” — along the coordinate axes.

For this purpose we have studied the following cases (see figure 1) for the region  $\mathcal{R}$  (for a reason to be clarified later all the needles start from a site whose distance from the origin is two: for example the needle along the positive  $z$ -axis will start from the site with coordinate  $(0, 0, 2)$ ):

- 1) a needle along one direction;
- 2) two needles along the positive and negative directions of an axis;
- 3) two needles along two different axes;

- 4) four needles in a plane along the two directions of two axes;
- 5) three needles along three different axes;
- 6) six needles along the two directions of all the three axes.

Notice that in the last case it is necessary that the needles start from a point located at distance two from the origin, otherwise the SAW starting from the origin would necessarily touch one of the needles.

Let us now define a few observables which will allow us to study the effect of the introduction of the excluded region. If  $(x, y, z)$  are the coordinates of the end-point of the SAW (or, equivalently,  $(r, \theta, \phi)$  in polar coordinates) a natural choice of observables is given by  $r^l Y_{l,m}(\theta, \phi)$ ,  $l \neq 0$ , where  $Y_{l,m}(\theta, \phi)$  are the spherical harmonics. If  $\langle r^l Y_{l,m}(\theta, \phi) \rangle$  is not identically vanishing because of the residual cubic symmetry which survives the introduction of the excluded region, this quantity is a natural candidate for a direct determination of the exponent  $\Delta$ . Indeed, since the critical limit is rotational-invariant, the leading term for  $N \rightarrow \infty$ , i.e.  $A(k)$  in formula (2.7), will vanish and thus this quantity will scale as  $N^{\nu-\Delta}$ .

Let us now classify the various observables according to the value of  $l$ . For  $l = 1$  the possibilities are

$$r(Y_{1,1}(\theta, \phi) + Y_{1,-1}(\theta, \phi)) \sim x \quad (3.1)$$

$$r(Y_{1,1}(\theta, \phi) - Y_{1,-1}(\theta, \phi)) \sim y \quad (3.2)$$

$$rY_{1,0}(\theta, \phi) \sim z \quad (3.3)$$

We can thus define  $O_1(x) = x$  and the obvious permutations. This observable is useful whenever the region  $\mathcal{R}$  is not invariant under the inversion of the  $x$ -axis.

Let us now consider  $l = 2$ . In this case we have

$$r^2(Y_{2,2}(\theta, \phi) + Y_{2,-2}(\theta, \phi)) \sim x^2 - y^2 \quad (3.4)$$

$$r^2(Y_{2,2}(\theta, \phi) - Y_{2,-2}(\theta, \phi)) \sim xy \quad (3.5)$$

$$r^2(Y_{2,1}(\theta, \phi) + Y_{2,-1}(\theta, \phi)) \sim xz \quad (3.6)$$

$$r^2(Y_{2,1}(\theta, \phi) - Y_{2,-1}(\theta, \phi)) \sim yz \quad (3.7)$$

$$r^2Y_{2,0}(\theta, \phi) \sim x^2 + y^2 - 2z^2 \quad (3.8)$$

We can thus define three observables

$$O_{2,1}(x, y) = x^2 - y^2 \quad (3.9)$$

$$O_{2,2}(x, y) = xy \quad (3.10)$$

$$O_{2,3}(x, y) = z^2 - \frac{1}{2}(x^2 + y^2) \quad (3.11)$$

It is clear that, whenever a symmetry between two axes exists, the two variables  $O_{2,1}$  and  $O_{2,3}$  are equivalent. In our calculation we have thus only considered the last two quantities.

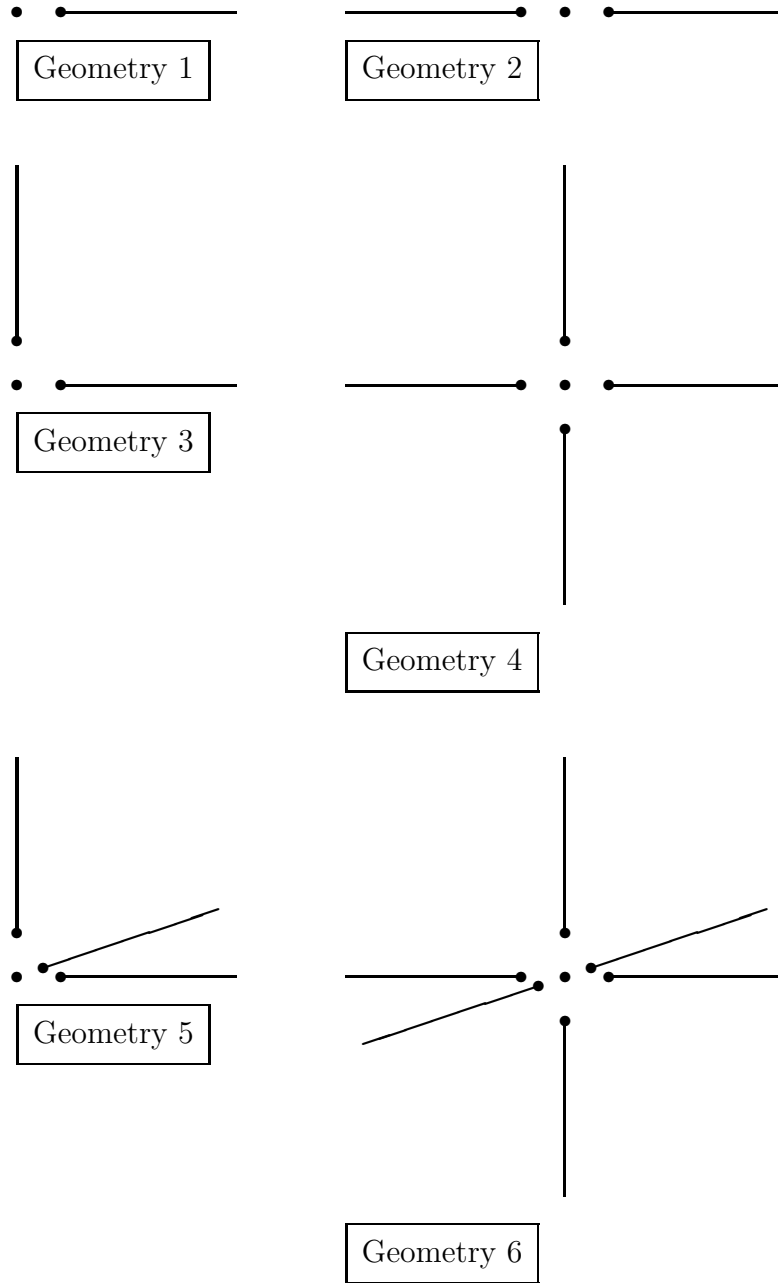


Figure 1: The six different geometries we have simulated. For each geometry we have reported as a dot the starting point of the walk (located at the origin) and the starting points of the excluded needles (located at distance two from the origin).



We have finally considered  $l = 4$ . In this case many different observables can be defined. We have only considered

$$O_{4,1} = \frac{2}{3} [x^4 + y^4 + z^4 - 3(x^2y^2 + x^2z^2 + y^2z^2)] \quad (3.12)$$

$$O_{4,2}(x) = x^4 + \frac{1}{2} (y^4 + z^4) - 3x^2 (y^2 + z^2) \quad (3.13)$$

Notice that when the excluded region is symmetric under any exchange of two axes  $O_{4,1}$  and  $O_{4,2}$  are equivalent. It is also worth remarking that  $O_{4,1}$  and  $O_{4,2}$  do not vanish even in absence of any excluded region, as they are invariant under the full cubic group.

Let us now define exactly our observables for the various geometries:

1. geometry 1 [needle along the positive  $x$ -axis]: we measure  $O_1 \equiv O_1(x)$ ,  $O_2 \equiv O_{2,3}(y, z)$  and  $O_4 \equiv O_{4,2}(x)$ ;
2. geometry 2 [two needles along the  $x$ -axis]: we measure  $O_2 \equiv O_{2,3}(y, z)$  and  $O_4 \equiv O_{4,2}(x)$ ;
3. geometry 3 [two needles along the positive  $x$ - and  $y$ -axis]: we measure  $O_1 \equiv \frac{1}{2}(O_1(x) + O_1(y))$ ,  $O_2 \equiv \frac{1}{2}(O_{2,3}(y, z) + O_{2,3}(z, x)) = -\frac{1}{2}O_{2,3}(x, y)$ ,  $\tilde{O}_2 \equiv O_{2,2}(x, y)$  and  $O_4 \equiv O_{4,1}$ ;
4. geometry 4 [four needles in the  $xy$ -plane]: we measure  $O_2 \equiv \frac{1}{2}(O_{2,3}(y, z) + O_{2,3}(z, x)) = -\frac{1}{2}O_{2,3}(x, y)$  and  $O_4 \equiv \frac{1}{2}(O_{4,2}(x) + O_{4,2}(y))$ ;
5. geometry 5 [three needles along three different axes]: we measure  $O_1 \equiv \frac{1}{3}(O_1(x) + O_1(y) + O_1(z))$ ,  $\tilde{O}_2 \equiv \frac{1}{3}(O_{2,2}(x, y) + O_{2,2}(x, z) + O_{2,2}(x, y))$  and  $O_4 \equiv O_{4,1}$ ;
6. geometry 6 [six needles]: we measure  $O_4 \equiv O_{4,1}$ .

## 4 The Monte Carlo simulation

### 4.1 Monte Carlo observables

The purpose of our simulation was to compute the mean values of the observables we have defined in the previous Section in presence of an excluded region  $\mathcal{R}$ . A direct strategy would be to simulate SAWs in presence of the region  $\mathcal{R}$  and then to compute the mean values of the various observables in the usual way. However this strategy requires different simulations for different excluded regions  $\mathcal{R}$ . To avoid repeating the runs many times we have simulated SAWs without any excluded region and then we have reweighted the results in order to obtain the mean values of interest. Since, as we have previously discussed, the introduction of the excluded region is an irrelevant perturbation, this strategy does not introduce any significant loss of efficiency.

Let us suppose we want to compute  $\langle \mathcal{O} \rangle_{N,\mathcal{R}}$  where  $\langle \cdot \rangle_{N,\mathcal{R}}$  indicates the ensemble of SAWs of length  $N$  that do not intersect the region  $\mathcal{R}$ . Then we simply use

$$\langle \mathcal{O} \rangle_{N,\mathcal{R}} = \frac{\langle \mathcal{O} \theta^{(\mathcal{R})} \rangle_N}{\langle \theta^{(\mathcal{R})} \rangle_N} \quad (4.1)$$

where  $\langle \cdot \rangle_N$  indicates the average in the ensemble of all SAWs of length  $N$  and  $\theta^{(\mathcal{R})}$  is an observable which assumes the value one if a walk does not intersect  $\mathcal{R}$  and zero otherwise. Notice moreover that  $\langle \theta^{(\mathcal{R})} \rangle_N$  gives also the probability  $p_{\mathcal{R}}$  that a SAW intersects the excluded region as  $p_{\mathcal{R}} = 1 - \langle \theta^{(\mathcal{R})} \rangle_N$ .

We have used (4.1) to obtain from our simulation the mean values  $\langle \mathcal{O} \rangle_{N,\mathcal{R}}$ : indeed it is enough, beside measuring at each Monte Carlo step  $i$  the value  $\mathcal{O}_i$ , to record  $\theta_i^{(\mathcal{R})}$  which assumes the value one if the walk intersects  $\mathcal{R}$ , zero otherwise and then estimate  $\langle \mathcal{O} \rangle_{N,\mathcal{R}}$  by

$$\frac{\sum_{i=1}^n \mathcal{O}_i \theta_i^{(\mathcal{R})}}{\sum_{i=1}^n \theta_i^{(\mathcal{R})}} \quad (4.2)$$

In order to further reduce the variance of our estimates we have also symmetrized our observables. To clarify the method suppose we want to compute  $\langle \mathcal{O}_1 \rangle_{N,\mathcal{R}}$  for geometry 1 ( $\mathcal{R}$  is the positive  $x$ -axis). We could consider

$$\frac{\langle x \theta^{(+x)} \rangle_N}{\langle \theta^{(+x)} \rangle_N} \quad (4.3)$$

A symmetrized alternative is

$$\frac{\langle x(\theta^{(+x)} - \theta^{(-x)}) + y(\theta^{(+y)} - \theta^{(-y)}) + z(\theta^{(+z)} - \theta^{(-z)}) \rangle_N}{\langle \theta^{(+x)} + \theta^{(-x)} + \theta^{(+y)} + \theta^{(-y)} + \theta^{(+z)} + \theta^{(-z)} \rangle_N} \quad (4.4)$$

It is obvious that this quantity has the same mean value of the previous one. However this symmetrization reduces the error on the estimates essentially at no computational cost. Indeed, since we study all six geometries at the same time, we must check in any case if the walk intersects any of the axes.

In general, given a geometry  $\mathcal{R}$  we have considered all the possible sets  $s_{\mathcal{R}}$  of excluded needles which can be obtained by all the transformations of the cubic group (six for geometry 1, three for geometry 2, twelve for geometry 3, three for geometry 4, eight for geometry 5, one for geometry 6). To each region  $s_{\mathcal{R}}$  we associate a variable  $\theta^{(s_{\mathcal{R}})}$ , which is one if the walk does not intersect the set  $s_{\mathcal{R}}$ , zero otherwise and  $\mathcal{O}^{(s_{\mathcal{R}})}$  which is the suitably transformed variable. Then we compute  $\langle \mathcal{O} \rangle_{N,\mathcal{R}}$  from

$$\langle \mathcal{O} \rangle_{N,\mathcal{R}} = \frac{\langle \sum_{\{s_{\mathcal{R}}\}} \theta^{(s_{\mathcal{R}})} \mathcal{O}^{(s_{\mathcal{R}})} \rangle}{\langle \sum_{\{s_{\mathcal{R}}\}} \theta^{(s_{\mathcal{R}})} \rangle} \quad (4.5)$$

The symmetrization has a large effect on the static variances of the various observables. For instance consider for each geometry the ratio

$$R = \frac{\text{var } \theta^{\mathcal{R}}}{\text{var } \frac{1}{n_{\mathcal{R}}} \sum \theta^{(s_{\mathcal{R}})}} \quad (4.6)$$

where “var” indicates the static variance and  $n_{\mathcal{R}}$  is the number of terms in the sum. We find  $R = 6.6, 3.2, 3.8, 2.7, 1.8, 1$  in the six geometries, which represents a considerable improvement. The improvement on the error bars is however not so large as the symmetrized observables are more correlated than the unsymmetrized ones. Thus the error bars are only 20-30% better.

To conclude let us comment briefly on the determination of the error bars. From a Monte Carlo run of  $n$  iterations we have estimated  $\langle O \rangle_{N,\mathcal{R}}$  using

$$\langle O \rangle_{N,\mathcal{R}} = \frac{\overline{\sum_{\{s_{\mathcal{R}}\}} \theta^{(s_{\mathcal{R}})} O^{(s_{\mathcal{R}})}}}{\overline{\sum_{\{s_{\mathcal{R}}\}} \theta^{(s_{\mathcal{R}})}}} \quad (4.7)$$

where, as usual  $\overline{\mathcal{O}} = \frac{1}{n} \sum_i \mathcal{O}_i$ . To compute the error bars one must take into account the correlation between the numerator and the denominator: the independent error formula indeed overestimates the true error bar. For  $O_1$  the difference is of about 20–30%, for  $O_2$  and  $\tilde{O}_2$  of 4–7%, while for  $O_4$  the difference is negligible. We have thus used the following relation, valid in the large sample limit,

$$\text{Var} \left( \frac{\overline{\sum_{\{s_{\mathcal{R}}\}} \theta^{(s_{\mathcal{R}})} O^{(s_{\mathcal{R}})}}}{\overline{\sum_{\{s_{\mathcal{R}}\}} \theta^{(s_{\mathcal{R}})}}} \right) = \frac{\langle \sum_{\{s_{\mathcal{R}}\}} \theta^{(s_{\mathcal{R}})} O^{(s_{\mathcal{R}})} \rangle^2}{\langle \sum_{\{s_{\mathcal{R}}\}} \theta^{(s_{\mathcal{R}})} \rangle^2} \text{Var}(\mathcal{A}). \quad (4.8)$$

where  $\mathcal{A}$  is given by

$$\mathcal{A} = \frac{\sum_{\{s_{\mathcal{R}}\}} \theta^{(s_{\mathcal{R}})} O^{(s_{\mathcal{R}})}}{\langle \sum_{\{s_{\mathcal{R}}\}} \theta^{(s_{\mathcal{R}})} O^{(s_{\mathcal{R}})} \rangle} - \frac{\sum_{\{s_{\mathcal{R}}\}} \theta^{(s_{\mathcal{R}})}}{\langle \sum_{\{s_{\mathcal{R}}\}} \theta^{(s_{\mathcal{R}})} \rangle} \quad (4.9)$$

The variance of  $\mathcal{A}$  has been computed using the standard techniques of autocorrelation analysis [28, 27]. Since the autocorrelation function has a very long tail (due to the fact that  $\tau_{exp} \sim N/f \gg \tau_{int,X}$  where  $f$  is the acceptance fraction of the algorithm and  $X$  a generic *global* observable), the self-consistent windowing method proposed in [28] does not work. Indeed even using a large window of  $40\tau_{int,\mathcal{A}}$ , the autocorrelation time is largely underestimated. To get a reliable estimate of  $\tau_{int}$  we have used the recipe proposed in the Appendix of [27]. We compute  $\tau_{int,X}$  by

$$\tau'_{int,X}(M) = \frac{1}{2} + \sum_{t=1}^M \rho_X(t) \quad (4.10)$$

$$\tau_{int,X} = \tau'_{int,X}(M) + \rho_X(M) M \log \left( \frac{N}{Mf} \right) \quad (4.11)$$

where  $\rho_X(t)$  is the normalized autocorrelation function,  $N$  the length of the walk,  $f$  the acceptance fraction;  $M$  is determined self-consistently and is the smallest integer such that  $20\tau'_{int,X}(M) > M$ . We have checked the *ad hoc* definition (4.11) in the case

		standard pivot	improved pivot
geometry	observable	$\tau_{int}$	$\tau_{int}$
1	$O_1$	$6.92 \pm 0.23$	$1.4869 \pm 0.0030$
	$p_{\mathcal{R}}$	$282 \pm 60$	$5.381 \pm 0.013$
2	$p_{\mathcal{R}}$	$280 \pm 60$	$5.026 \pm 0.011$
3	$O_1$	$7.73 \pm 0.27$	$1.4946 \pm 0.0030$
	$p_{\mathcal{R}}$	$307 \pm 68$	$5.081 \pm 0.012$
4	$p_{\mathcal{R}}$	$311 \pm 69$	$4.2485 \pm 0.0083$
5	$O_1$	$8.58 \pm 0.32$	$1.4293 \pm 0.0029$
	$p_{\mathcal{R}}$	$312 \pm 70$	$4.628 \pm 0.010$
6	$p_{\mathcal{R}}$	$261 \pm 53$	$2.7910 \pm 0.0048$

Table 1: Autocorrelation times for the pivot algorithm and our improvement for the observables  $O_1$  (in the geometries where it does not vanish) and  $p_{\mathcal{R}}$ . Here  $N = 1000$ .

of ordinary random walks for which exact results are available [28]: the error in the estimation of the tail turns out to be at most 10%. We have thus set the error bars on the autocorrelation times adding to the error in the determination of  $\tau'_{int,X}(M)$ , one tenth of the last term in (4.11).

## 4.2 The algorithm

We have simulated SAWs of fixed length  $N$  in three dimensions without any excluded region  $\mathcal{R}$ . The walk is given by  $N + 1$  lattice points  $\{\omega_i\}$ ,  $i = 0, \dots, N$ , and always starts from the origin, i.e.  $\omega_0 = 0$ . Since all our observables are completely symmetric under the cubic group, it is not restrictive to fix the first step; we have chosen  $\omega_1 = (1, 0, 0)$ .

The simulation used the *pivot* algorithm [29, 30, 28]. In the standard implementation a site  $\omega_k$  in the walk and an element  $g$  of the lattice symmetry group are chosen randomly, with uniform probability. The proposed configuration, obtained from the actual one by applying  $g$  to the part of the walk subsequent to  $\omega_k$ , is accepted whenever self-avoiding. This algorithm is extraordinarily efficient for the study of global observables like, for example, the end-point position; indeed, the integrated autocorrelation time for these observables grows with the number  $N$  of steps in the walk like  $N^p$ , where  $p \approx 0.11$  in  $d = 3$ , while the CPU-time to produce an independent walk scales like  $N$  which is the optimal situation.

However in our case not all the observables are of global character: an example is the probability of intersection  $p_{\mathcal{R}}$ . Indeed, as can be seen from table 1, already at  $N = 1000$ ,  $\tau_{int,p_{\mathcal{R}}} \approx 300$ . It is easy to understand the origin of these autocorrelation times: indeed suppose the walk intersects  $\mathcal{R}$  and let  $\alpha$  be the smallest integer such that  $\omega_\alpha \in \mathcal{R}$ . Then all subsequent walks in the simulation will also intersect  $\mathcal{R}$  at

least until a successful pivot move at point  $i$  with  $i < \alpha$  is performed. The probability of such a move is  $\alpha f/N$  where  $f$  is the acceptance fraction. Now the problem is that the typical  $\alpha$  is very small: if one considers the set of walks that intersect at least one of the six needles of the geometry 6, the mean value of the smallest  $\alpha$  such that  $\omega_\alpha \in \mathcal{R}$  is  $\approx 13$ , with very small  $N$ -dependent corrections. Thus a rough estimate of the autocorrelation times should be  $N/(13f)$ . For  $N = 1000$  we have  $f \approx 0.45$  so that we expect  $\tau \approx 200$  which is indeed the order of magnitude we find. Moreover we expect  $\tau$  to increase as  $N^{\approx 1}$  as it should for local observables. Indeed we find that  $\tau$  for  $p_{\mathcal{R}}$  increases as  $N^p$  with  $p \approx 0.9$  except in the case of geometry 6 where we observe  $p \approx 0.6$ , which could however well be an effective exponent in the region  $500 \leq N \leq 32000$ .

The other observables, like  $O_1$ , are instead of more global character and indeed the autocorrelation times are much smaller<sup>3</sup>. They also increase more slowly with  $N$ ; for  $O_1$  we find  $\tau_{int,O_1} \sim N^{\approx 0.3}$ .

To eliminate these long autocorrelation times one must increase the frequency of the moves with the first points of the walk as pivots. We have thus modified the algorithm in the following way: one iteration consists now of the following three moves:

- one move with pivot point in  $\omega_1$ :
- one move with pivot point  $\omega_k$  with  $k$  uniformly chosen in the interval  $1 < k \leq 13$ ;
- one move with pivot point  $\omega_k$  with  $k$  uniformly chosen in the interval  $13 < k \leq N - 1$ .

With this improvement, the autocorrelation times, are greatly reduced. Table 1 contains a comparison between autocorrelation time for the two algorithms for walks of length  $N_{tot} = 1000$ . We observed sensible reductions of autocorrelation times for each observable, but the most impressive results are obtained for the observable  $p_{\mathcal{R}}$ , which denotes the fraction of walks that intersect the considered excluded set. To compare CPU-times one should notice that one iteration of the improved algorithm takes three times the CPU-time of an iteration of the standard algorithm. Thus in practice use of the improved algorithm allowed us to gain a factor of 15 – 20 on  $p_{\mathcal{R}}$  (although no improvement on the exponent  $p$ ) and a factor 1.5 – 2 on global observables like  $O_1$ .

## 5 The results

We have studied SAWs with length  $500 \leq N \leq 32000$ . The number of iterations for each value of  $N$  is reported in table 2. The total simulation required 2500 hours of

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<sup>3</sup>When we speak of autocorrelation time for  $O_1$  we really intend the  $\tau_{int,\mathcal{A}}$  as defined in (4.9) as this is the observable which controls the error on  $O_1$ .

	500	1000	2000	4000	8000	16000	32000
$N_{iter.}$	$3 \cdot 10^7$	$5 \cdot 10^7$	$6 \cdot 10^7$	$7 \cdot 10^7$	$1 \cdot 10^8$	$5 \cdot 10^7$	$2 \cdot 10^7$

Table 2: Number of iterations.

CPU on a AlphaStation 600 Mod 5/266. We have computed  $\Delta$  studying the quantities we have previously discussed, whose leading behaviour for  $N \rightarrow \infty$  is

$$\langle O_k \rangle_N = B_{\mathcal{R}}(k) N^\sigma \quad (5.1)$$

where  $\sigma = k\nu - \Delta$ ,  $k = 1, 2, 4$ . We have performed standard power-law fits neglecting the next subleading terms. This introduces a systematic error which in our case could be particularly serious due to small value of  $\Delta$ . Indeed one expects corrections to (5.1) of the form  $N^{k\nu-2\Delta}$  which decay very slowly and could thus give sizable corrections even at the relatively large values of  $N$  we use. To get an idea of the systematic error we have repeated the fits using each time only those values of  $N$  satisfying  $N \geq N_{cut}$ . In this way one gets different estimates which should converge to  $\Delta$  as  $N_{cut}$  goes to infinity. If the different estimates are essentially independent of  $N_{cut}$  (within error bars) one can reasonably trust the estimate of  $\Delta$ , otherwise one gets an idea of the size of the systematic error.

We show the results of our fits for each geometry in Tables 3–8. In the first column one can find the different values of  $N_{cut}$ , in the second one the raw Monte Carlo data, in the next one the estimated value of the exponent and finally the confidence level of the fit. In the last column we report the “classical prediction” for the exponent  $\sigma$ , obtained using (2.8). In the computation of the expectation values we used the estimate for  $\nu$  given by [27]

$$\nu = 0.5877 \pm 0.0006 \quad (5.2)$$

Let us now comment on the results. Let us consider first the observable  $O_1$ . Since the estimates for  $N_{cut} \geq 4000$  are essentially constant within error bars one could estimate

$$\sigma = \begin{cases} 0.396(3) & \text{for geometry 1} \\ 0.388(3) & \text{for geometry 3} \\ 0.379(3) & \text{for geometry 5} \end{cases} \quad (5.3)$$

These estimates have very small statistical error bars. However the fact that the estimates do not agree within the stated errors is a clear indication that there is a much larger error due to the neglected corrections to scaling. Indeed a closer look to the data shows that in all cases there is still an upward trend, although not statistically significant as the change of  $\sigma$  is smaller than the error bars. It is thus more cautious to interpret the results for  $\sigma$  as lower bounds on the true value. Thus we estimate  $\sigma = 0.39 \gtrsim 0.01$  and thus  $\Delta \lesssim 0.20 \pm 0.01$ .

Let us now consider the observable  $O_2$ . This quantity shows much larger corrections to scaling compared to the previous one: indeed in no case we can identify a

geometry 1					
	cut	$\langle O \rangle \pm \delta\langle O \rangle$	$\sigma \pm \delta\sigma$	$CL$	
$O_1$	500	$-1.5259 \pm 0.0014$	$0.40044 \pm 0.00044$	$9 \cdot 10^{-7}\%$	$\nu - \Delta =$ $1 - \nu =$ $0.4123 \pm 0.0006$
	1000	$-2.0229 \pm 0.0018$	$0.39831 \pm 0.00060$	0.114%	
	2000	$-2.6751 \pm 0.0028$	$0.39584 \pm 0.00091$	14.118%	
	4000	$-3.5322 \pm 0.0044$	$0.3932 \pm 0.0016$	62.627%	
	8000	$-4.6324 \pm 0.0060$	$0.3955 \pm 0.0029$	92.618%	
	16000	$-6.092 \pm 0.015$	$0.3962 \pm 0.0080$		
	32000	$-8.018 \pm 0.040$			
$O_2$	500	$-20.457 \pm 0.047$	$0.97813 \pm 0.00098$	$29 \cdot 10^{-4}\%$	$2\nu - \Delta = 1$
	1000	$-39.944 \pm 0.089$	$0.9818 \pm 0.0013$	3.622%	
	2000	$-78.25 \pm 0.20$	$0.9859 \pm 0.0020$	53.836%	
	4000	$-155.00 \pm 0.43$	$0.9866 \pm 0.0031$	35.367%	
	8000	$-306.42 \pm 0.85$	$0.9908 \pm 0.0054$	26.964%	
	16000	$-606.0 \pm 3.0$	$1.005 \pm 0.014$		
	32000	$-1217. \pm 10.$			
$O_4$	500	$(-110 \pm 11) \cdot 10^2$	$2.277 \pm 0.035$	15.228%	$4\nu - \Delta =$ $1 + 2\nu =$ $2.1754 \pm 0.0012$
	1000	$(-596 \pm 50) \cdot 10^2$	$2.239 \pm 0.044$	20.112%	
	2000	$(-295 \pm 25) \cdot 10^3$	$2.182 \pm 0.063$	22.338%	
	4000	$(-160 \pm 12) \cdot 10^4$	$2.056 \pm 0.096$	51.065%	
	8000	$(-642 \pm 53) \cdot 10^4$	$2.10 \pm 0.20$	25.931%	
	16000	$(-304 \pm 41) \cdot 10^5$	$1.43 \pm 0.62$		
	32000	$(-82 \pm 34) \cdot 10^6$			

Table 3: One excluded needle. Here  $CL$  denotes the confidence level of the fit.

geometry 2					
	cut	$\langle O \rangle \pm \delta\langle O \rangle$	$\sigma \pm \delta\sigma$	$CL$	
$O_2$	500	$-45.97 \pm 0.11$	$0.9622 \pm 0.0010$	$22 \cdot 10^{-5} \%$	$2\nu - \Delta = 1$
	1000	$-88.71 \pm 0.20$	$0.9664 \pm 0.0014$	1.206%	
	2000	$-171.86 \pm 0.46$	$0.9712 \pm 0.0021$	32.894%	
	4000	$-336.7 \pm 1.0$	$0.9732 \pm 0.0034$	23.052%	
	8000	$-658.2 \pm 2.0$	$0.9801 \pm 0.0060$	33.624%	
	16000	$-1292.7 \pm 6.9$	$0.994 \pm 0.016$		
	32000	$-2575. \pm 25.$			
$O_4$	500	$(-299 \pm 12) \cdot 10^2$	$2.206 \pm 0.015$	11.869%	$4\nu - \Delta =$ $1 + 2\nu =$ $2.1754 \pm 0.0012$
	1000	$(-1437 \pm 50) \cdot 10^2$	$2.190 \pm 0.019$	14.368%	
	2000	$(-670 \pm 25) \cdot 10^3$	$2.162 \pm 0.028$	15.761%	
	4000	$(-328 \pm 12) \cdot 10^4$	$2.099 \pm 0.045$	39.275%	
	8000	$(-1374 \pm 54) \cdot 10^4$	$2.122 \pm 0.085$	18.371%	
	16000	$(-634 \pm 40) \cdot 10^5$	$1.80 \pm 0.26$		
	32000	$(-221 \pm 37) \cdot 10^6$			

Table 4: Two opposite needles. Here  $CL$  denotes the confidence level of the fit.

geometry 3					
	cut	$\langle O \rangle \pm \delta\langle O \rangle$	$\sigma \pm \delta\sigma$	$CL$	
$O_1$	500	$-1.6573 \pm 0.0015$	$0.39267 \pm 0.00044$	$4 \cdot 10^{-8} \%$	$\nu - \Delta$ $1 - \nu =$ $0.4123 \pm 0.0006$
	1000	$-2.1859 \pm 0.0020$	$0.39038 \pm 0.00060$	0.037%	
	2000	$-2.8761 \pm 0.0030$	$0.38767 \pm 0.00092$	13.770%	
	4000	$-3.7761 \pm 0.0048$	$0.3850 \pm 0.0016$	59.748%	
	8000	$-4.9246 \pm 0.0065$	$0.3873 \pm 0.0029$	70.556%	
	16000	$-6.436 \pm 0.016$	$0.3901 \pm 0.0081$		
	32000	$-8.435 \pm 0.042$			
$O_2$	500	$-10.696 \pm 0.025$	$0.9717 \pm 0.0010$	$5 \cdot 10^{-5} \%$	$2\nu - \Delta = 1$
	1000	$-20.740 \pm 0.047$	$0.9761 \pm 0.0013$	2.063%	
	2000	$-40.42 \pm 0.11$	$0.9809 \pm 0.0020$	55.682%	
	4000	$-79.86 \pm 0.24$	$0.9811 \pm 0.0034$	35.520%	
	8000	$-157.19 \pm 0.45$	$0.9859 \pm 0.0057$	31.462%	
	16000	$-309.9 \pm 1.6$	$1.000 \pm 0.015$		
	32000	$-619.8 \pm 5.6$			
$\tilde{O}_2$	500	$-0.1650 \pm 0.0081$	$0.772 \pm 0.036$	5.684%	$2\nu - \Delta = 1$
	1000	$-0.276 \pm 0.016$	$0.730 \pm 0.057$	4.327%	
	2000	$-0.572 \pm 0.035$	$0.512 \pm 0.092$	89.526%	
	4000	$-0.819 \pm 0.079$	$0.53 \pm 0.18$	74.224%	
	8000	$-1.07 \pm 0.18$	$0.77 \pm 0.43$	63.693%	
	16000	$-2.02 \pm 0.67$	$0.1 \pm 1.4$		
	32000	$-2.2 \pm 2.0$			
$O_4$	500	$(-166 \pm 12) \cdot 10^2$	$2.244 \pm 0.025$	10.182%	$4\nu - \Delta =$ $1 + 2\nu =$ $2.1754 \pm 0.0012$
	1000	$(-864 \pm 52) \cdot 10^2$	$2.211 \pm 0.032$	16.821%	
	2000	$(-414 \pm 25) \cdot 10^3$	$2.171 \pm 0.046$	17.299%	
	4000	$(-214 \pm 12) \cdot 10^4$	$2.071 \pm 0.072$	40.820%	
	8000	$(-871 \pm 54) \cdot 10^4$	$2.10 \pm 0.14$	18.912%	
	16000	$(-409 \pm 42) \cdot 10^5$	$1.56 \pm 0.44$		
	32000	$(-120 \pm 34) \cdot 10^6$			

Table 5: Two needles along two different axes. Here  $CL$  denotes the confidence level of the fit.



geometry 4					
	cut	$\langle O \rangle \pm \delta \langle O \rangle$	$\sigma \pm \delta \sigma$	$CL$	
$O_2$	500	$-25.876 \pm 0.071$	$0.9439 \pm 0.0012$	$10^{-7}\%$	$2\nu - \Delta = 1$
	1000	$-49.00 \pm 0.13$	$0.9501 \pm 0.0016$	$0.747\%$	
	2000	$-93.52 \pm 0.29$	$0.9561 \pm 0.0024$	$34.436\%$	
	4000	$-182.09 \pm 0.63$	$0.9552 \pm 0.0040$	$19.884\%$	
	8000	$-351.1 \pm 1.2$	$0.9643 \pm 0.0072$	$35.181\%$	
	16000	$-682.1 \pm 4.1$	$0.981 \pm 0.020$		
	32000	$-1347. \pm 17.$			
$O_4$	500	$(-518 \pm 13) \cdot 10^2$	$2.1760 \pm 0.0099$	$3.475\%$	$4\nu - \Delta$ $1 + 2\nu =$ $2.1754 \pm 0.0012$
	1000	$(-2425 \pm 55) \cdot 10^2$	$2.161 \pm 0.013$	$6.562\%$	
	2000	$(-1104 \pm 27) \cdot 10^3$	$2.142 \pm 0.019$	$7.781\%$	
	4000	$(-521 \pm 14) \cdot 10^4$	$2.094 \pm 0.031$	$24.042\%$	
	8000	$(-2181 \pm 61) \cdot 10^4$	$2.1083 \pm 0.057$	$9.664\%$	
	16000	$(-991 \pm 42) \cdot 10^5$	$1.86 \pm 0.16$		
	32000	$(-359 \pm 37) \cdot 10^6$			

Table 6: Four needles in a plane. Here  $CL$  denotes the confidence level of the fit.

geometry 5					
	cut	$\langle O \rangle \pm \delta \langle O \rangle$	$\sigma \pm \delta \sigma$	$CL$	
$O_1$	500	$-1.8113 \pm 0.0017$	$0.38443 \pm 0.00045$	$13 \cdot 10^{-10}\%$	$\nu - \Delta =$ $1 - \nu =$ $0.4123 \pm 0.0006$
	1000	$-2.3764 \pm 0.0022$	$0.38193 \pm 0.00061$	$0.012\%$	
	2000	$-3.1097 \pm 0.0034$	$0.37900 \pm 0.00093$	$12.449\%$	
	4000	$-4.0587 \pm 0.0053$	$0.3762 \pm 0.0016$	$55.622\%$	
	8000	$-5.2613 \pm 0.0073$	$0.3786 \pm 0.0030$	$58.046\%$	
	16000	$-6.833 \pm 0.016$	$0.3828 \pm 0.0082$		
	32000	$-8.909 \pm 0.046$			
$\tilde{O}_2$	500	$-0.1892 \pm 0.0088$	$0.763 \pm 0.034$	$3.242\%$	$2\nu - \Delta = 1$
	1000	$-0.311 \pm 0.017$	$0.732 \pm 0.052$	$2.100\%$	
	2000	$-0.645 \pm 0.038$	$0.518 \pm 0.084$	$81.853\%$	
	4000	$-0.952 \pm 0.086$	$0.50 \pm 0.17$	$63.392\%$	
	8000	$-1.20 \pm 0.17$	$0.79 \pm 0.39$	$61.993\%$	
	16000	$-2.27 \pm 0.66$	$0.2 \pm 1.3$		
	32000	$-2.5 \pm 2.2$			
$O_4$	500	$(-282 \pm 12) \cdot 10^2$	$2.211 \pm 0.016$	$5.575\%$	$4\nu - \Delta =$ $1 + 2\nu =$ $2.1754 \pm 0.0012$
	1000	$(-1393 \pm 53) \cdot 10^2$	$2.188 \pm 0.021$	$10.689\%$	
	2000	$(-649 \pm 26) \cdot 10^3$	$2.159 \pm 0.030$	$11.283\%$	
	4000	$(-321 \pm 13) \cdot 10^4$	$2.088 \pm 0.048$	$30.950\%$	
	8000	$(-1334 \pm 54) \cdot 10^4$	$2.103 \pm 0.089$	$12.901\%$	
	16000	$(-618 \pm 42) \cdot 10^5$	$1.73 \pm 0.26$		
	32000	$(-205 \pm 35) \cdot 10^6$			

Table 7: Three needles along three different axes. Here  $CL$  denotes the confidence level of the fit.

geometry 6					
	cut	$\langle O \rangle \pm \delta \langle O \rangle$	$\sigma \pm \delta \sigma$	$CL$	
$O_4$	500	$(-787 \pm 16) \cdot 10^2$	$2.1540 \pm 0.0086$	4.443%	$4\nu - \Delta =$ $1 + 2\nu =$ $2.1754 \pm 0.0012$
	1000	$(-3606 \pm 67) \cdot 10^2$	$2.141 \pm 0.011$	7.879%	
	2000	$(-1611 \pm 35) \cdot 10^3$	$2.123 \pm 0.017$	9.185%	
	4000	$(-746 \pm 17) \cdot 10^4$	$2.078 \pm 0.028$	33.022%	
	8000	$(-3093 \pm 76) \cdot 10^4$	$2.097 \pm 0.053$	15.301%	
	16000	$(-1382 \pm 56) \cdot 10^5$	$1.89 \pm 0.15$		
	32000	$(-513 \pm 50) \cdot 10^6$			

Table 8: Six needles along the two directions of all the three axes. Here  $CL$  denotes the confidence level of the fit.

region of  $N_{cut}$  where the estimates are constant. In all cases the estimates of  $\sigma$  are clearly increasing with  $N_{cut}$ . Using the results with  $N_{cut} = 8000$  we have

$$\sigma \gtrsim \begin{cases} 0.991(5) & \text{for geometry 1} \\ 0.980(6) & \text{for geometry 2} \\ 0.986(6) & \text{for geometry 3} \\ 0.964(7) & \text{for geometry 4} \end{cases} \quad (5.4)$$

We conclude thus that  $\sigma \gtrsim 0.99 \pm 0.01$  so that  $\Delta \lesssim 0.19 \pm 0.01$ .

Consider now the observable  $O_4$ . It has much larger errors than the two previous ones. Here we can only give a very rough estimate  $\sigma \approx 2.10(10)$  so that  $\Delta \approx 0.25(10)$ .

Finally let us discuss the results for  $\tilde{O}_2$ . In this case the estimates of  $\sigma$  are much lower than expected and indeed for both geometries 3 and 5 they seem to indicate, although without much confidence,  $\sigma \approx 0.5 \pm 0.2$ . It thus appears that this observable does not couple to the leading operator breaking the rotational invariance. This fact can be proved rigorously for the ordinary random walk: in Appendix A we show that for geometries 3 and 5 we have indeed

$$\langle \tilde{O}_2 \rangle_N = 0 \quad (5.5)$$

for all values of  $N$ . For the SAW  $\langle \tilde{O}_2 \rangle_N \neq 0$ ; however our data show that for this observable, in formula (2.7), not only  $A$  but also  $B_{\mathcal{R}}$  vanishes. Thus the study of  $\langle \tilde{O}_2 \rangle_N$  allows to compute a new subleading exponent  $\Delta' > \Delta$ : from  $\sigma \sim 0.5$  we would get  $\Delta' \sim 0.7$ . Notice however that the error bars are too big to really trust this estimate.

Let us now discuss the behaviour of the intersection probabilities  $p_{\mathcal{R}}$ . As discussed before, pure dimensional arguments suggest that the probability that a SAW intersects any one-dimensional set is vanishing in a three-dimensional space. This argument works of course in the *continuum* limit. For SAWs on the lattice this statement translates in the fact that given a SAW of length  $N$ ,  $\{\omega_i\}_{i=0,\dots,N}$ , and a

geometry	cut	$p_{\mathcal{R}} \pm \delta p_{\mathcal{R}}$	$\Delta \pm \delta\Delta$	$CL$
1	500	$0.182995 \pm 0.000067$	$0.2150 \pm 0.0064$	74.926%
	1000	$0.194002 \pm 0.000070$	$0.215 \pm 0.012$	58.808%
	2000	$0.203434 \pm 0.000089$	$0.223 \pm 0.026$	40.621%
	4000	$0.21173 \pm 0.00012$	$0.16 \pm 0.13$	56.695%
	8000	$0.21861 \pm 0.00014$		
	16000	$0.22461 \pm 0.00027$		
	32000	$0.23041 \pm 0.00058$		
2	500	$0.34624 \pm 0.00012$	$0.2357 \pm 0.0067$	83.318%
	1000	$0.36415 \pm 0.00012$	$0.234 \pm 0.013$	69.572%
	2000	$0.37928 \pm 0.00015$	$0.237 \pm 0.027$	48.991%
	4000	$0.39235 \pm 0.00019$	$0.176 \pm 0.052$	61.677%
	8000	$0.40309 \pm 0.00022$		
	16000	$0.41235 \pm 0.00044$		
	32000	$0.42116 \pm 0.00094$		
3	500	$0.33456 \pm 0.00011$	$0.2276 \pm 0.0063$	74.457%
	1000	$0.35209 \pm 0.00011$	$0.226 \pm 0.012$	58.934%
	2000	$0.36696 \pm 0.00014$	$0.232 \pm 0.026$	39.799%
	4000	$0.37993 \pm 0.00018$	$0.168 \pm 0.086$	54.075%
	8000	$0.39061 \pm 0.00021$		
	16000	$0.39983 \pm 0.00041$		
	32000	$0.40874 \pm 0.00088$		
4	500	$0.58302 \pm 0.00015$	$0.2637 \pm 0.0067$	75.629%
	1000	$0.60509 \pm 0.00015$	$0.259 \pm 0.013$	64.062%
	2000	$0.62332 \pm 0.00018$	$0.258 \pm 0.027$	43.116%
	4000	$0.63875 \pm 0.00023$	$0.195 \pm 0.064$	55.552%
	8000	$0.65123 \pm 0.00025$		
	16000	$0.66182 \pm 0.00047$		
	32000	$0.6718 \pm 0.0010$		
5	500	$0.46027 \pm 0.00013$	$0.2397 \pm 0.0063$	72.307%
	1000	$0.48113 \pm 0.00013$	$0.236 \pm 0.012$	58.015%
	2000	$0.49865 \pm 0.00016$	$0.242 \pm 0.025$	38.594%
	4000	$0.51380 \pm 0.00021$	$0.177 \pm 0.072$	53.900%
	8000	$0.52619 \pm 0.00024$		
	16000	$0.53683 \pm 0.00046$		
	32000	$0.5470 \pm 0.0010$		
6	500	$0.74526 \pm 0.00016$	$0.2897 \pm 0.0068$	49.055%
	1000	$0.76491 \pm 0.00014$	$0.280 \pm 0.012$	49.324%
	2000	$0.78069 \pm 0.00017$	$0.276 \pm 0.024$	30.554%
	4000	$0.79389 \pm 0.00019$	$0.206 \pm 0.052$	57.904%
	8000	$0.80432 \pm 0.00020$		
	16000	$0.81312 \pm 0.00035$		
	32000	$0.82126 \pm 0.00067$		

Table 9: Probabilities of intersection  $p_{\mathcal{R}}$  for the various geometries. Here  $CL$  denotes the confidence level of the fit used to determine  $\Delta$ .

one-dimensional set  $S$  such that  $\omega_0$  is at a distance of order  $N^\nu$  from  $S$ , then the probability that the walk intersects  $S$  goes to zero for  $N \rightarrow \infty$  as  $N^{-\Delta}$ . In our case  $p_{\mathcal{R}}$  is however the probability that the SAW intersects a one-dimensional set  $\mathcal{R}$  which is at a finite fixed distance from the origin of the walk. In this case we expect the intersection probability to tend to a constant as  $N \rightarrow \infty$  and thus a behaviour of the form

$$p_{\mathcal{R}}(N) = p_{\mathcal{R}}(\infty) + \frac{b_{\mathcal{R}}}{N^\Delta} \quad (5.6)$$

The results for  $p_{\mathcal{R}}$  for the various geometries are reported in Table 9, together with the estimates of  $\Delta$  from a three-parameter fit of the form (5.6). The estimates indicate  $\Delta = 0.23(3)$  except for the geometry 6 in which case one would derive a much higher value of  $\Delta$ ,  $\Delta \approx 0.28$ . These discrepancies should not however be taken seriously: the fit (5.6) is very unstable in presence of additional subleading corrections. To understand the size of the systematic error one should expect from fits of the form (5.6), we have performed the following test: we have considered  $O_1$  and we have analyzed the data as

$$\frac{\langle O_1 \rangle_N}{N^\nu} = a + bN^{-\Delta} \quad (5.7)$$

where we have used  $\nu = 0.5877$ . In all cases we have obtained estimates  $\Delta \approx 0.16 - 0.23$  and moreover we have found  $a$  barely compatible with zero within error bars (for instance for the geometry 1,  $N_{cut} = 4000$ , we have  $a = (24 \pm 23) \cdot 10^{-4}$ ). Clearly the additional corrections play still an important role. It is however reassuring that the value of  $\Delta$  is in essential agreement with what we expect.

## 6 Conclusions

In this paper we have studied the role played by one-dimensional vacancies in the critical behaviour of the three-dimensional SAW. As already pointed out in [1, 2] a new critical exponent arises. We have carefully checked that the exponent depends only on the dimensionality of the vacancies by verifying its independence from the shape of the excluded region: in particular it does not depend on the discrete symmetry which the lattice has after the introduction of the excluded region.

We have given a geometrical argument to interpret the new exponent and we have thus derived a classical prediction for it. Of course we expect renormalization effects to change the classical formula: we will thus write

$$\Delta = 2\nu - 1 + \eta_{\mathcal{R}} \approx 0.175 + \eta_{\mathcal{R}} \quad (6.1)$$

The quantity  $\eta_{\mathcal{R}}$  is an anomalous dimension which is expected to be small. Our numerical data give

$$\Delta = 0.18 \pm 0.02 \quad (6.2)$$

so that  $|\eta_{\mathcal{R}}| \lesssim 0.02$ . The classical prediction, obtained setting  $\eta_{\mathcal{R}} = 0$  is thus a very good approximation.

Let us notice that our estimate of  $\Delta$  is somewhat lower than the estimate of [1],  $\Delta \approx 0.24$  and of [2],  $\Delta \approx 0.217 \pm 0.013$ . The origin of these discrepancies is probably

in the neglected additional corrections to scaling: the results of [1] are obtained from an exact enumeration and thus probe only very short walks, while the estimate of [2] comes from walks which have mainly  $N \approx 1000 - 4000$ . Here we use longer SAWs and a much higher statistics and thus we can do a much more detailed study of the role of the next subleading terms. We thus hope to have a better control of the additional corrections although it is conceivable that also our present estimate is systematically higher than the true result. We hope that our error bar, which we believe is very conservative, takes correctly into account these systematic effects.

Let us finally remark that all the arguments we have given are of extremely general nature and can thus be used for other systems and geometries.

## A Critical behaviour of random walks in presence of $d_{\mathcal{R}}$ dimensional vacancies

Consider a  $d$ -dimensional lattice  $\Omega$  and a region  $\mathcal{R}$ . Then let  $c_N(x)$  be the number of ordinary random walks, starting from the origin and ending in  $x$ , that never intersect  $\mathcal{R}$  except for  $t = 0$ . In this appendix we will derive a general integral equation for the generating function which can be solved exactly when  $\mathcal{R}$  is a  $d_{\mathcal{R}}$ -dimensional hyperplane. In this way we will be able to check the computations of Section 2.

Let us start from the recursion relations

$$\begin{aligned} c_0(x) &= \delta(x, 0) \quad , \\ c_N(x) &= \sum_{i=1}^d [c_{N-1}(x + e_i) + c_{N-1}(x - e_i)] \cdot \left(1 - \sum_{\alpha \in \mathcal{R}} \delta(x, \alpha)\right) \quad \text{for } N \geq 1 \end{aligned} \quad (\text{A.1})$$

where  $e_i$  is the unit vector in the  $i$ -direction. Let us now introduce the generating function

$$G(x) = \sum_{N=0}^{\infty} \beta^N c_N(x) \quad (\text{A.2})$$

and its Fourier transform  $\hat{G}(q)$ . It is then a simple matter to obtain the following equation

$$\begin{aligned} \hat{G}(q) &= 1 + \beta \hat{G}(q) (2d - \hat{q}^2) \\ &\quad - \beta \int_{-\pi}^{\pi} \frac{d^d k}{(2\pi)^d} \hat{G}(k) (2d - \hat{k}^2) \sum_{\alpha \in \mathcal{R}} e^{i(k-q) \cdot \alpha} \end{aligned} \quad (\text{A.3})$$

where  $\hat{q}_i = 2 \sin\left(\frac{q_i}{2}\right)$ . Define now the free propagator which coincides (apart from a factor  $\beta$ ) with the generating function for unconstrained random walks

$$D(q) = \frac{1}{m_0^2 + \hat{q}^2} = \frac{\beta}{1 - 2\beta \sum_{i=1}^d \cos q_i} \quad (\text{A.4})$$

where  $m_0^2 = \frac{1-2\beta d}{\beta}$ . Then (A.3) can be rewritten as

$$\hat{G}(q) = \frac{1}{\beta} D(q) - D(q) \int_{-\pi}^{\pi} \frac{d^d k}{(2\pi)^d} \hat{G}(k) (2d - \hat{k}^2) \sum_{\alpha \in \mathcal{R}} e^{i(k-q) \cdot \alpha} \quad (\text{A.5})$$

This equation is completely general and applies to any excluded region  $\mathcal{R}$ .

Let us now restrict ourselves to the case in which  $\mathcal{R}$  is the  $d_{\mathcal{R}}$ -dimensional hyperplane given by the equations  $x_{d_{\mathcal{R}+1}} = \dots = x_d = 0$ . If we now multiply (A.5) by  $(2d - \hat{q}^2) \sum_{\eta \in \mathcal{R}} e^{i(q-k') \cdot \eta}$  and integrate over  $q$ , using the identity  $2d - \hat{q}^2 = \frac{1}{\beta} - D(q)^{-1}$ , we obtain

$$\begin{aligned} \int_{-\pi}^{\pi} \frac{d^d q}{(2\pi)^d} \hat{G}(q) (2d - \hat{q}^2) \sum_{\alpha \in \mathcal{R}} e^{i(q-k') \cdot \alpha} = \\ \frac{1}{\beta} \left[ 1 - \beta \left( \int_{-\pi}^{\pi} \frac{d^d q}{(2\pi)^d} D(q) \sum_{\alpha \in \mathcal{R}} e^{i(q-k') \cdot \alpha} \right)^{-1} \right] \end{aligned} \quad (\text{A.6})$$

Inserting back in (A.5) we get finally

$$\hat{G}(q) = \frac{D(q)}{\int_{-\pi}^{\pi} \frac{d^{\mathcal{D}_{\mathcal{R}} k}}{(2\pi)^{\mathcal{D}_{\mathcal{R}}}} D(q_1, \dots, q_{d_{\mathcal{R}}}, k_{d_{\mathcal{R}+1}}, \dots, k_d)} \quad (\text{A.7})$$

where  $\mathcal{D}_{\mathcal{R}} = d - d_{\mathcal{R}}$ . It is easy to check that this solution has the correct properties. Indeed one can verify immediately that  $G(x) = \delta_{x,0}$  whenever  $x \in \mathcal{R}$ . Notice finally that for  $d_{\mathcal{R}} = 0$  the solution does not become the standard solution for unconstrained random walks, but gives the generating function for random walks with the excluded origin.

Let us now consider the critical limit  $m_0 \rightarrow 0$  and let us define

$$\begin{aligned} I_{\mathcal{R}}(\hat{m}_0^2) &\equiv \int_{-\pi}^{\pi} \frac{d^{\mathcal{D}_{\mathcal{R}} k}}{(2\pi)^{\mathcal{D}_{\mathcal{R}}}} D(q_1, \dots, q_{d_{\mathcal{R}}}, k_{d_{\mathcal{R}+1}}, \dots, k_d) = \\ &\int_{-\pi}^{\pi} \frac{d^{\mathcal{D}_{\mathcal{R}} k}}{(2\pi)^{\mathcal{D}_{\mathcal{R}}}} \frac{1}{\hat{m}_0^2 + \hat{k}^2} \end{aligned} \quad (\text{A.8})$$

where  $\hat{m}_0^2 = m_0^2 + \hat{q}_{\parallel}^2$  and  $q_{\parallel} = (q_1, \dots, q_{d_{\mathcal{R}}}, 0, \dots, 0)$ . The introduction of the excluded region will thus be relevant or irrelevant depending on the behaviour of  $I(\hat{m}_0^2)$  for  $\hat{m}_0 \rightarrow 0$ . If the limit exists the perturbation is irrelevant, while if the integral diverges the perturbation is relevant or marginal. This last case corresponds to  $\mathcal{D}_{\mathcal{R}} = 1, 2$ . For  $\mathcal{D}_{\mathcal{R}} = 1$ , we have

$$I_{\mathcal{R}}(\hat{m}_0^2) = \frac{1}{\hat{m}_0 \sqrt{\hat{m}_0^2 + 4}} \quad (\text{A.9})$$

and the critical behaviour is drastically changed since

$$\hat{G}(q) = \frac{\sqrt{m_0^2 + \hat{q}_{\parallel}^2} \sqrt{m_0^2 + \hat{q}_{\parallel}^2 + 4}}{m_0^2 + \hat{q}^2} . \quad (\text{A.10})$$

In the critical limit we have

$$\hat{G}(q) = \frac{2\sqrt{m_0^2 + q_{\parallel}^2}}{m_0^2 + q^2} . \quad (\text{A.11})$$

From this expression it is easy to verify that, for  $N \rightarrow \infty$ ,

$$c_N \equiv \sum_x c_N(x) \approx \frac{2}{\sqrt{2\pi d}} (2d)^N N^{-1/2} \quad (\text{A.12})$$

so that  $\gamma = 1/2$  which differs from the value of  $\gamma$  for random walks in free space,  $\gamma = 1$ . Analogously we have

$$\langle x_1^2 \rangle_N \approx \frac{N}{d} , \quad (\text{A.13})$$

$$\langle x_d^2 \rangle_N \approx \frac{2N}{d} . \quad (\text{A.14})$$

The exponent  $\nu$  is not changed, but the amplitudes are, as expected, dependent on the direction and different from the value they assume in free space,  $\langle x_1^2 \rangle_N = \langle x_d^2 \rangle_N = N/d$ .

If  $\mathcal{D}_{\mathcal{R}} = 2$ , which, as we shall see, corresponds to a marginal operator, we have

$$I_{\mathcal{R}}(\hat{m}_0^2) = \frac{2}{\pi} \frac{1}{\hat{m}_0^2 + 4} K\left(\frac{4}{\hat{m}_0^2 + 4}\right) \quad (\text{A.15})$$

where  $K(z)$  is an elliptic integral. For  $\hat{m}_0^2 \rightarrow 0$ ,  $I_{\mathcal{R}}(\hat{m}_0^2)$  diverges logarithmically so that we get in the critical limit

$$\hat{G}(q) = -\frac{4\pi}{(m_0^2 + q^2) \log[(m_0^2 + q_{\parallel}^2)/32]} \quad (\text{A.16})$$

Thus the propagator differs from the unperturbed one only by a logarithmic correction. From this expression we easily get

$$c_N \equiv \sum_x c_N(x) \sim \frac{(2d)^N}{\log N} . \quad (\text{A.17})$$

Thus in this case we have  $\gamma = 1$  as for random walks in free space: however an additional logarithmic correction appears as expected in the marginal case. Analogously we find

$$\langle x_1^2 - x_d^2 \rangle_N \sim \frac{N}{\log N} . \quad (\text{A.18})$$

If now  $\mathcal{D}_{\mathcal{R}} > 2$   $I_{\mathcal{R}}(\hat{m}_0^2)$  has a finite limit for  $\hat{m}_0 \rightarrow 0$  so that in the critical limit

$$\hat{G}(q) = \frac{D(q)}{I_{\mathcal{R}}(0)} \quad (\text{A.19})$$

Thus  $\hat{G}(q)$  is identical to the generating function of unconstrained random walks except for a multiplicative constant which is related to the total number of walks  $c_N = \sum_x c_N(x)$ . Indeed from (A.19) it follows that for large  $N$

$$c_N \approx \frac{(2d)^N}{2dI_{\mathcal{R}}(0)} \quad (\text{A.20})$$

so that  $p_{\mathcal{R}}$ , the probability that an unconstrained random walk intersects  $\mathcal{R}$  is simply  $1 - 1/(2dI_{\mathcal{R}}(0))$ . It is easy to check that this probability tends to zero as  $d \rightarrow \infty$  at  $d_{\mathcal{R}}$  fixed. Indeed, let us compute the large- $\mathcal{D}_{\mathcal{R}}$  expansion of  $I_{\mathcal{R}}(0)$ : we start from the standard representation of  $I_{\mathcal{R}}(m_0^2)$  in terms of Bessel functions:

$$I_{\mathcal{R}}(\hat{m}_0^2) = \int_0^\infty dt e^{-t(\hat{m}_0^2 + 2\mathcal{D}_{\mathcal{R}})} I_0^{\mathcal{D}_{\mathcal{R}}}(2t) \quad (\text{A.21})$$

where  $I_0(t)$  is the zeroth-order Bessel function of first kind. Expanding  $I_0(t)$  around  $t = 0$  we get finally

$$I_{\mathcal{R}}(\hat{m}_0^2) = \frac{1}{\hat{m}_0^2 + 2\mathcal{D}_{\mathcal{R}}} \times \sum_{n_1=0}^\infty \cdots \sum_{n_{\mathcal{D}_{\mathcal{R}}}=0}^\infty \frac{(2n_1 + \cdots + 2n_{\mathcal{D}_{\mathcal{R}}})!}{(n_1! \cdots n_{\mathcal{D}_{\mathcal{R}}}!)^2} \frac{1}{(\hat{m}_0^2 + 2\mathcal{D}_{\mathcal{R}})^{2(n_1 + \cdots + n_{\mathcal{D}_{\mathcal{R}}})}} \quad (\text{A.22})$$

so that, for  $\mathcal{D}_{\mathcal{R}} \rightarrow \infty$ ,

$$I_{\mathcal{R}}(0) \approx \frac{1}{2\mathcal{D}_{\mathcal{R}}} \left( 1 + \frac{1}{2\mathcal{D}_{\mathcal{R}}} + \frac{3}{4\mathcal{D}_{\mathcal{R}}^2} + \cdots \right) \quad (\text{A.23})$$

It follows that for  $d \rightarrow \infty$ ,  $p_{\mathcal{R}} \approx (2d_{\mathcal{R}} + 1)/(2d)$ .

Let us now discuss the subleading corrections to (A.19). We need here the small- $\hat{m}_0^2$  expansion of  $I(\hat{m}_0^2)$ . We start from the well-known asymptotic expansion for large  $t$  of the Bessel function  $I_0(2t)$

$$I_0^{\mathcal{D}_{\mathcal{R}}}(2t) \approx e^{2\mathcal{D}_{\mathcal{R}}t} \sum_{n=0}^\infty \frac{b_n(\mathcal{D}_{\mathcal{R}})}{(2t)^{\frac{\mathcal{D}_{\mathcal{R}}}{2}+n}} \quad (\text{A.24})$$

Using (A.21) we can rewrite our integral as

$$\begin{aligned} I_{\mathcal{R}}(\hat{m}_0^2) &\approx \int_0^1 dt e^{-t\hat{m}_0^2} \left[ e^{-2t} I_0(2t) \right]^{\mathcal{D}_{\mathcal{R}}} + \\ &\int_1^\infty dt e^{-t\hat{m}_0^2} \left[ \left( e^{-2t} I_0(2t) \right)^{\mathcal{D}_{\mathcal{R}}} - \sum_{n=0}^\infty \frac{b_n(\mathcal{D}_{\mathcal{R}})}{(2t)^{\frac{\mathcal{D}_{\mathcal{R}}}{2}+n}} \right] + \\ &\int_1^\infty dt e^{-t\hat{m}_0^2} \sum_{n=0}^\infty \frac{b_n(\mathcal{D}_{\mathcal{R}})}{(2t)^{\mathcal{D}_{\mathcal{R}}/2+n}} \end{aligned} \quad (\text{A.25})$$

The first two integrals have a regular expansion in terms of powers of  $\hat{m}_0^2$ .



Let us now determine the behaviour in  $\hat{m}_0^2$  of the generic term appearing in the series in the last term. Integrating by parts we get

$$\begin{aligned} \int_1^\infty dt e^{-t\hat{m}_0^2} \frac{b_n(\mathcal{D}_{\mathcal{R}})}{(2t)^{\mathcal{D}_{\mathcal{R}}/2+n}} &= \frac{\hat{m}_0^{\mathcal{D}_{\mathcal{R}}+2n-2}}{2^{\mathcal{D}_{\mathcal{R}}/2+n}} b_n(\mathcal{D}_{\mathcal{R}}) \int_{\hat{m}_0^2}^\infty d\xi \frac{e^{-\xi}}{\xi^{\mathcal{D}_{\mathcal{R}}/2+n}} = \\ &= \frac{b_n(\mathcal{D}_{\mathcal{R}})}{2^{\mathcal{D}_{\mathcal{R}}/2+n}} \left\{ \left[ \sum_{l=1}^{g(k,n)} \hat{m}_0^{2l-2} (-1)^{l-1} \left( \prod_{i=1}^l \frac{1}{\mathcal{D}_{\mathcal{R}}/2+n-i} \right) \right] \left[ \sum_{s=0}^\infty \frac{(-1)^s}{s!} \hat{m}_0^{2s} \right] + \right. \\ &\quad \left. (-1)^{g(k,n)} \hat{m}_0^{\mathcal{D}_{\mathcal{R}}+2n-2} F(\hat{m}_0^2) \left( \prod_{i=1}^{g(k,n)} \frac{1}{\mathcal{D}_{\mathcal{R}}/2+n-i} \right) \right\} \end{aligned} \quad (\text{A.26})$$

where, for  $k$  integer,

$$g(k, n) = \begin{cases} k+n-1 & \text{if } \mathcal{D}_{\mathcal{R}} = 2k; \\ k+n+1 & \text{if } \mathcal{D}_{\mathcal{R}} = 2k+1 \end{cases} \quad (\text{A.27})$$

$$F(\hat{m}_0^2) = \begin{cases} -\text{Ei}(-\hat{m}_0^2) = -\log \hat{m}_0^2 - \gamma_E - \sum_{k=1}^\infty \frac{(-1)^k \hat{m}_0^{2k}}{k \cdot k!} & \text{if } \mathcal{D}_{\mathcal{R}} = 2k; \\ \frac{\sqrt{\pi}}{2} - \hat{m}_0^3 \sum_{k=0}^\infty \frac{(-1)^k \hat{m}_0^{2k}}{(k+\frac{3}{2}) \cdot k!} & \text{if } \mathcal{D}_{\mathcal{R}} = 2k+1 \end{cases} \quad (\text{A.28})$$

Here  $\gamma_E$  is the Euler-Mascheroni constant,  $\gamma_E \approx 0.5772156649$ . The whole integral can be represented in terms of  $\hat{m}_0^2$  by

$$I_{\mathcal{R}}(\hat{m}_0^2) = \sum_{n=0}^\infty A_n \hat{m}_0^{2n} + \hat{m}_0^{\mathcal{D}_{\mathcal{R}}-2} C(\hat{m}_0^2) ; \quad (\text{A.29})$$

$A_n$  are suitable constants and  $C(\hat{m}_0^2)$  is a function of  $\hat{m}_0^2$  which is finite for  $\hat{m}_0^2 \rightarrow 0$  for  $\mathcal{D}_{\mathcal{R}}$  odd, diverging logarithmically for  $\mathcal{D}_{\mathcal{R}}$  even. The second term in (A.29) represents the effect of the excluded region and corresponds to an exponent  $\Delta$

$$\Delta = \nu(\mathcal{D}_{\mathcal{R}} - 2) = \frac{1}{2} \mathcal{D}_{\mathcal{R}} - 1 \quad (\text{A.30})$$

which agrees with our prediction.

To conclude this appendix let us prove a result for more general excluded regions which we will use in the main text. Let the excluded region be of the form  $\mathcal{R} = \cup_{i=1}^d \mathcal{R}_i$  where  $\mathcal{R}_i$  is some subset of points of the  $i$ -th coordinate axis. If  $i_1 \neq i_2 \dots \neq i_n$ ,  $2 \leq n \leq d$ , then

$$\langle x_{i_1} x_{i_2} \dots x_{i_n} \rangle_N = 0 \quad (\text{A.31})$$

In particular, for geometries 3 and 5 we have  $\langle \tilde{O}_2 \rangle_N = 0$ .

To prove (A.31) consider (A.5), which, as we already said, is valid for general excluded regions  $\mathcal{R}$ . Using now

$$\left. \frac{\partial}{\partial q_{i_1}} \frac{\partial}{\partial q_{i_2}} \dots \frac{\partial}{\partial q_{i_n}} D(q) \right|_{q=0} = 0 \quad (\text{A.32})$$

$$\frac{\partial}{\partial q_{i_1}} \frac{\partial}{\partial q_{i_2}} \dots \frac{\partial}{\partial q_{i_n}} \sum_{\alpha \in \mathcal{R}} e^{i(k-q) \cdot \alpha} = 0 \quad (\text{A.33})$$

$N$	$\langle x^2 + y^2 + z^2 \rangle_N$	$\langle x^4 + y^4 + z^4 \rangle_N$	$Q_N$
500	$1785.8 \pm 1.1$	$(28727 \pm 38) \cdot 10^2$	$0.90078 \pm 0.00046$
1000	$4051.8 \pm 2.0$	$(14826 \pm 16) \cdot 10^3$	$0.90309 \pm 0.00039$
2000	$9167.4 \pm 4.4$	$(76027 \pm 81) \cdot 10^3$	$0.90464 \pm 0.00038$
4000	$20752.9 \pm 9.4$	$(38994 \pm 39) \cdot 10^4$	$0.90539 \pm 0.00036$
8000	$46995 \pm 18$	$(20020 \pm 17) \cdot 10^5$	$0.90649 \pm 0.00032$
16000	$106166 \pm 60$	$(10222 \pm 13) \cdot 10^6$	$0.90692 \pm 0.00047$
32000	$240356 \pm 221$	$(5247 \pm 11) \cdot 10^7$	$0.90829 \pm 0.00078$

Table 10: Mean values for SAWs in absence of any excluded region.  $(x, y, z)$  are the coordinates of the end-point of the walk.

for  $i_1 \neq i_2 \dots \neq i_n$ ,  $2 \leq n \leq d$ , we get

$$\left. \frac{\partial}{\partial q_{i_1}} \frac{\partial}{\partial q_{i_2}} \dots \frac{\partial}{\partial q_{i_n}} \hat{G}(q) \right|_{q=0} = 0 \quad (\text{A.34})$$

from which (A.31) immediately follows.

## B Large-distance behaviour of the two-point function

In this Appendix we will present some results which concern the three-dimensional self-avoiding walk with no excluded region and we will use it to discuss, along the lines of [31, 23], the behaviour of the two-point function  $G(\vec{r}; \beta)$  in the large-distance region  $|r| \gtrsim R_e(\beta)$  where  $R_e(\beta)$  is the mean end-to-end distance. Consider now the Fourier transform  $\hat{G}(p; \beta)$ ; for  $\beta \rightarrow \beta_c = 1/\mu$  standard scaling theory predicts

$$\frac{\hat{G}(p; \beta)}{\hat{G}(0; \beta)} = \tilde{G}(q) \quad (\text{B.1})$$

where  $q = pR_e(\beta)/6$ . An important characteristic of  $\tilde{G}(q)$  is the fact that in the region  $q^2 \lesssim 1$ ,  $\tilde{G}(q)$  is essentially a free-field propagator, i.e. it can be parametrized as

$$\tilde{G}(q) \approx \frac{1}{1 + q^2} \quad (\text{B.2})$$

The deviations are small and can be parametrized by a  $(q^2)^2$  term, i.e. by

$$\tilde{G}(q) \approx \frac{1}{1 + q^2 + b_2(q^2)^2} \quad (\text{B.3})$$

A strong-coupling (exact-enumeration) study [23] set a bound on  $b_2$ :

$$-3 \cdot 10^{-4} \lesssim b_2 \lesssim 0 \quad . \quad (\text{B.4})$$

The constant  $b_2$  has also been computed [23] in the  $\epsilon$ -expansion and in the expansion in fixed dimension with the result :  $b_2 = -3 \cdot 10^{-4}$ .

Here we want to give a bound on  $b_2$  using our Monte Carlo data. A simple computation gives

$$b_2 = 1 - \frac{1}{2} \frac{\Gamma(\gamma)\Gamma(\gamma + 4\nu)}{\Gamma(\gamma + 2\nu)^2} Q \quad (\text{B.5})$$

where

$$Q = \lim_{N \rightarrow \infty} Q_N \equiv \lim_{N \rightarrow \infty} \frac{\langle x^4 + y^4 + z^4 \rangle_N}{\langle x^2 + y^2 + z^2 \rangle_N^2} \quad . \quad (\text{B.6})$$

Our Monte Carlo estimates for  $Q_N$  are reported in Table 10. It is evident that the data show strong corrections to scaling. To determine  $Q$  we have thus performed a fit of the form

$$Q_N = Q + \frac{A}{N^\Delta} \quad . \quad (\text{B.7})$$

We find

$$Q = 0.9091 \pm 0.0016 \quad , \quad (\text{B.8})$$

$$\Delta = 0.41 \pm 0.16 \quad , \quad (\text{B.9})$$

$$\chi^2 = 1.77 \quad (4 \text{ d.o.f.}) \quad . \quad (\text{B.10})$$

The value of  $\Delta$  is in agreement with the estimates of [27]. Using for  $\gamma$  the value [32]  $\gamma = 1.1575(5)$  we get finally

$$b_2 = -(13 \pm 17) 10^{-4} \quad . \quad (\text{B.11})$$

Our Monte Carlo data confirm the fact that  $b_2$  is extremely small although we are unable to compute the actual value.

On the other hand we can use (B.4) and (B.5) together with the estimates of  $\gamma$  and  $\nu$  to obtain an estimate of  $Q$ . We get  $Q = 0.9082(11)$ .

## References

- [1] D. Considine and S. Redner, J. Phys. **A22**, 1621 (1989).
- [2] S. Caracciolo, G. Ferraro and A. Pelissetto, J. Phys. **A24**, 3625 (1991).
- [3] P. Grassberger, J. Phys. **A26**, 2769 (1993).
- [4] M. Daoud, J. P. Cotton, B. Farnoux, G. Jannink, G. Sarma, H. Benoit, R. Duplessix, C. Picot and P. G. de Gennes, Macromolecules **8**, 804 (1975).
- [5] J. des Cloizeaux, J. Phys. (France) **36**, 281 (1975).

- [6] V. J. Emery, Phys. Rev. **B11**, 239 (1975).
- [7] C. Aragão de Carvalho, S. Caracciolo and J. Fröhlich, Nucl. Phys. **B215** [FS7], 209 (1983).
- [8] R. Fernández, J. Fröhlich and A. D. Sokal, *Random Walks, Critical Phenomena, and Triviality in Quantum Field Theory*, Text and Monographs in Physics (Springer-Verlag, Berlin, 1992).
- [9] J. des Cloizeaux and G. Jannink, *Polymers in solution: their Modelling and Structure* (Oxford, Clarendon Press, 1990).
- [10] J. M. Hammersley and S. G. Whittington, J. Phys. **A18**, 101 (1985).
- [11] F. Wegner, Phys. Rev. **B5**, 4529 (1972).
- [12] J. L. Cardy and S. Redner, J. Phys. **A17**, L933 (1984).
- [13] R. Z. Bariev, Zh. Eksp. Teor. Fiz. **77**, 1217 (1979); English translation Sov. Phys. JETP **50**, 613 (1979).
- [14] E. Eisenriegler and T. Burkhardt, Phys. Rev. **B24**, 1236 (1981).
- [15] K. Symanzik, Proc. Int. School of Physics “Enrico Fermi”, Varenna Course XLV, ed. R. Jost (Academic Press, 1969).
- [16] J. Fröhlich, Nucl. Phys. **B200** [FS4], 281 (1982).
- [17] G. Parisi, Phys. Lett. **B81**, 357 (1979).
- [18] M. E. Fisher, J. Stat. Phys. **34** 665 (1984).
- [19] D. A. Huse and M. E. Fisher, Phys. Rev. **B29** (1984) 239.
- [20] S. Mukherji and S. M. Bhattacharjee, J. Phys **A26**, L1139 (1995); J. Phys. **A28**, 4668 (1995) (E); Phys. Rev. **E48**, 3427 (1993); Phys. Rev. **E52**, 3301(E) (1995).
- [21] J. W. Essam and A. J. Guttmann, Phys. Rev. **E52**, 5849 (1995).
- [22] S. Caracciolo, A. Guttmann, B. Li, A. Pelissetto and A. D. Sokal, unpublished.
- [23] M. Campostrini, A. Pelissetto, P. Rossi and E. Vicari, `cond-mat/9612164` and in preparation.
- [24] G. A. Baker Jr., B. G. Nickel and D. I. Meiron, Phys. Rev. **B17**, 1365 (1978).
- [25] J. C. Le Guillou and J. Zinn-Justin, Phys. Rev. **B21**, 3976 (1980).
- [26] I. Majid, Z. V. Djordjevic and H. E. Stanley, Phys. Rev. Lett. **51**, 1282 (1983).
- [27] B. Li, N. Madras and A. D. Sokal, J. Stat. Phys. **80**, 661 (1995).

- [28] N. Madras and A. D. Sokal, J. Stat. Phys. **50**, 109 (1988).
- [29] M. Lal, Molec. Phys. **17**, 57 (1969).
- [30] B. MacDonald, N. Jan, D. L. Hunter and M. O. Steinitz, J. Phys. **A18**, 2627 (1985).
- [31] M. E. Fisher and A. A. Aharony, Phys. Rev. Lett. **31**, 1238 (1973); Phys. Rev. **B7**, 2818 (1974).
- [32] S. Caracciolo, M. S. Causo and A. Pelissetto, *High-precision determination of the critical exponent  $\gamma$  for self-avoiding walks*, preprint SNS/PH/1997-002, cond-mat/9703250 .